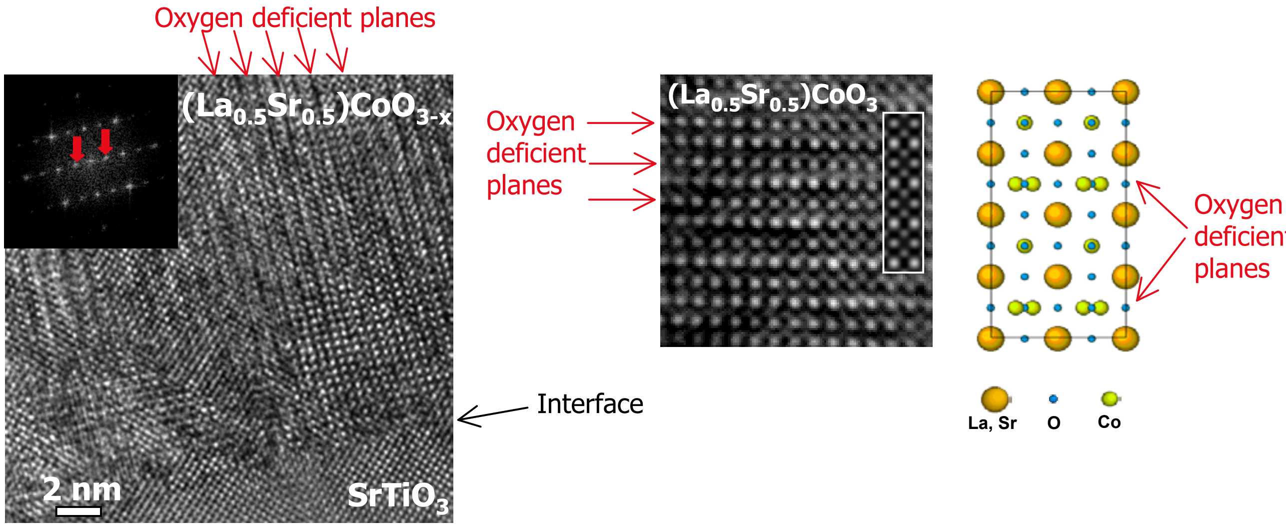
Interface Science of Functional Perovskites



Interface Science of Functional Perovskites: S. Stemmer (Rice University), DMR-009372. Functional, multicomponent oxides based on the perovskite structure exhibit properties as diverse as high-temperature superconductivity, fast oxygen transport, and sensing and actuating properties. As dimensions of these oxides are reduced to the nanoscale, the properties of these oxides are dominated by the properties of interfaces and surfaces. We are investigating the relationship between interfacial properties and structure, in particular related to the transport of oxygen across interfaces. For these studies, we synthesize thin films of these oxides with controlled orientations and interfaces. Oxygen transport in these oxides is governed by the arrangement and concentration of oxygen vacancies. In $(La_{0.5}Sr_{0.5})CoO_{3-x}$, one of our perovskite model materials, oxygen vacancies tend to form ordered arrangements. We can image these ordered structures in the electron microscope or analyze them by diffraction methods. We have discovered that the nature and alignment of ordering is governed by the substrate and by the nonstoichiometry of the film [J. Appl. Phys. 90(7), 3319-3324 (2001)]. For example, the left panel shows an ordered structure in a $(La_{0.5}Sr_{0.5})CoO_{3-x}$ film grown on a single crystal $SrTiO_3$. The oxygen deficient planes are arranged *perpendicular* to the substrate. Films grown on $LaAlO_3$ single crystals order with their oxygen deficient planes *parallel* to the substrate (middle panel). The image contrast observed in high-resolution electron microscopy is due to the relaxation of Co ions in the atom planes containing missing oxygen ions (oxygen is too weak a scatter to contribute to the contrast). Our model (right panel) of a oxygen deficient unit cell was confirmed by image simulation (inset in the middle panel), which matches the experimentally observed image contrast well. We are presently working on relating stress in the films with the vacancy ordered patterns. This is challenging, as the unstressed lattice parameters of the films are not known. The work will have significant impact on a number of areas. For example, it was shown that the film with the ordered structure in $LaAlO_3$ had a oxygen surface exchange coefficient orders of magnitude higher than a film with random arrangements. In collaboration with researchers at the University of Houston, we can now study transport and exchange properties along specific unit cell directions. Furthermore, oxygen vacancies also dominate the behavior of related materials, such as high temperature superconductors and ferroelectric perovskites.

Susanne Stemmer / Rice University / DMR-0093721: Interface Science of Functional Perovskites Diversity, Outreach and International Collaborative Activities

In addition to research, Prof. Stemmer's group at Rice University is involved a number of outreach and international activities. On February 19, 2002, Prof. Stemmer gave a lecture as part of an evening course for 9th-grade teachers of the Houston Independent School District's IPC (Integrated Physics and Chemistry Course) organized by the NSF funded Center for Nanosciences at Rice. Through a NSF-DAAD travel grant, a researcher (Dr. Keding) from the University of Jena (Germany) has visited Prof. Stemmer's group twice, and has interacted with the students funded by this project in an ongoing collaboration between the groups. Students funded by this grant during the past year included Jiwei Lu, a graduate student in Materials Science, and Jasmine Gipson, an undergraduate student in Materials Science. Ms. Gipson is an African American woman.